Polymer Information on STN
SLA - June 12

Session Agenda

- Polymer definition
- STN files with polymer information
- Polymers in CAS files
- Searching polymers in Registry
- Searching polymers in CAplus
- Polymer property information

What is a polymer?

- Polymers are large chemicals made up of smaller units (monomers) combined together to form chains
- Polymers may be natural or synthetic
- Plastics, rubbers, protein/nucleotide sequences, fibers, and adhesives are all polymers

Polymers on STN

- Scientific & Technical Information Network
- More than 200 databases in all areas
- Browser-based access available at http://stnweb.cas.org:

STN Files on Polymers

- **Chemical & Material Files:**
  - **CAplus, DKILIT, EMA, RAPRA, TEXTILETECH , WTEXTILES**
- **Substance Files**
  - **CHEMLIST, PDLCOM, PLASPEC, REGISTRY**
- **Property Files**
  - **ASMDATA, CAplus, DKILIT, PDLCOM, PLASPEC**

STN Files on Polymers

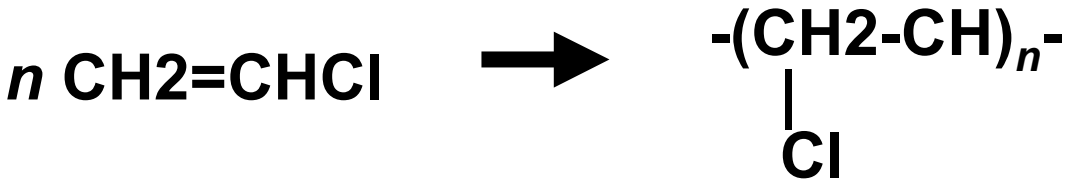
- **Business & News Files**
  - **CBNB, CEN, CIN, PLASNEWS, PROMT**
- **Patent Files**
  - **CAplus, IFIPAT, USPATFULL, USPAT2, WPIDS, WPINDEX**

Polymers in CAS Files

- World's largest and most current source of polymer information
- Indexing of synthetic polymers is usually based on monomers used to prepare them
- Supplemental indexing provided selectively for structure of the final polymer

Types of polymers

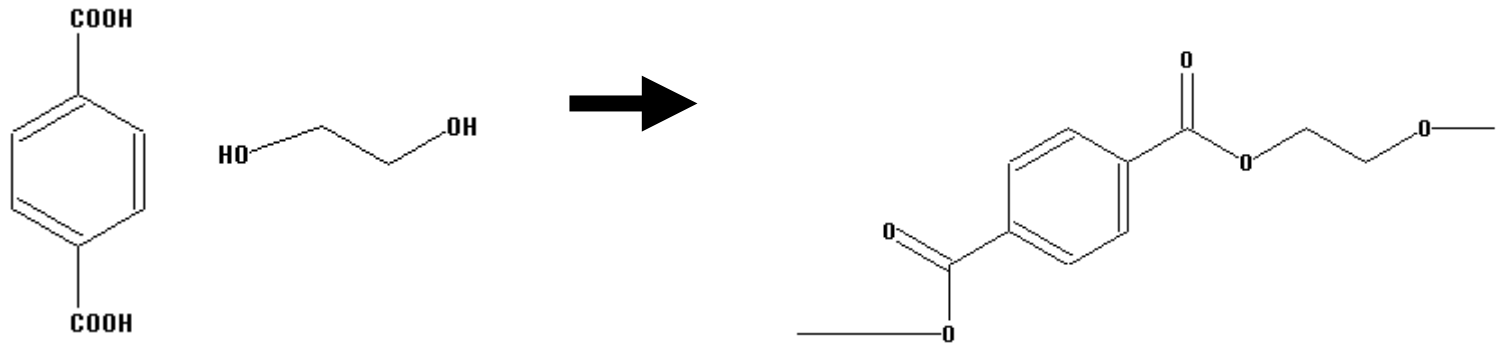
- **Addition (vinyl) polymerization**



  - **where *n*>10 or an unspecified number**
  - **monomer-based Registry Number only**

Types of polymers

- **Condensation polymerization**



  - **monomer-based Registry Number**
  - **supplemental Registry Number for structural repeating unit (SRU) if monomers are symmetrical**

Polymers in Registry

- The Registry file contains more than 928,038 polymeric substances (6/6/02)
- Registry is updated daily with new polymer entries
- Each polymer record is assigned an unique CAS Registry Number (RN)
- The RN can be used in bibliographic files to find corresponding references to the substance

Polymers in Registry

Factors that DO NOT affect polymer registration:

- **Molecular weight**
- **Monomer ratio in addition polymers**
  - **e.g., 60:40 and 90:10 ethylene-vinyl chloride copolymers have the same Registry Number**
- **Head-to-head versus head-to-tail arrangements**

Polymers in Registry

Factors that DO affect polymer registration:

- **Tacticity (stereochemistry)**
  - atactic polypropylene (NS) 9003-07-0
  - isotactic polypropylene 25085-53-4
  - syndiotactic polypropylene 26063-22-9
- **Presence of end-groups (SRU only)**
- **Block, graft, alternating polymer forms**
  - only since 1987

Registry Sample Record

```
L7    ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2002 ACS
RN    9003-53-6  REGISTRY
CN    Benzene, ethenyl-, homopolymer (9CI)
(CA INDEX NAME)
OTHER NAMES:
CN    105E
CN    138F
o  o  o
CN    Styrene homopolymer
ADDITIONAL NAMES NOT AVAILABLE IN THIS FORMAT
  - Use FCN, FIDE, or ALL for DISPLAY
MF    (C8 H8)x
CI    PMS, COM
PCT   Polystyrene
```

Other Names includes trade name designations and common names

Registry Record Continued

LC STN Files: ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, ASMDATA*, BIOBUSINESS, BIOSIS, BIOTECHNO,CA, CABA, CANCERLIT, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSCHEM, CSNB, DDFU, DETHERM*, DIOGENES, DRUGU, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE MSDS-OHS, NIOSHTIC, PDLCOM*, PHARMASEARCH, PIRA, PLASPEC*, PROMT, RTECS*, SPECINFO, TOXCENTER, TULSA, ULIDAT, USPAT2, USPATFULL, VTB

(*File contains numerically searchable property data)

Other Sources: DSL**, TSCA**

(**Enter CHEMLIST File for up-to-date regulatory information)

The Registry Number Locator field lists STN files that can be searched for information about the polymer

Registry Record Continued

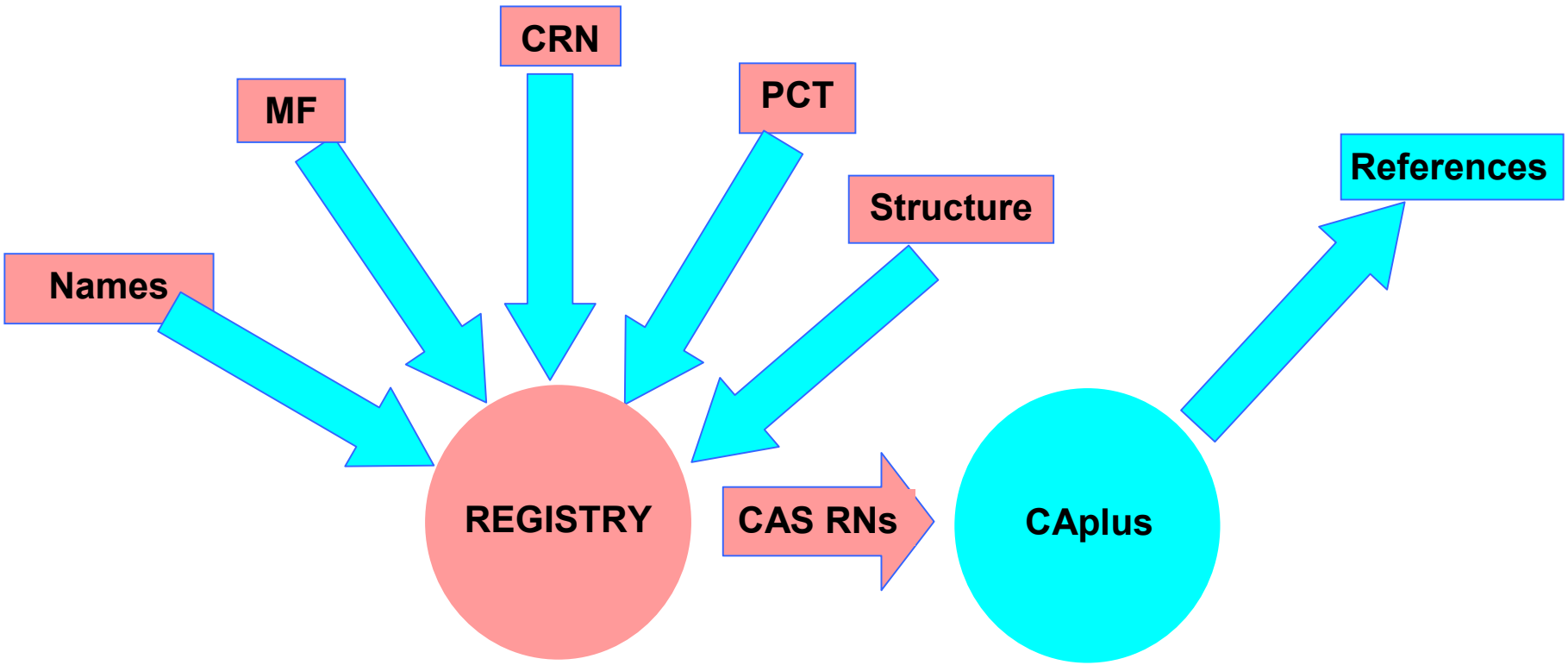
CM 1

CRN 100-42-5
CMF C8 H8

H2C=CH-Ph

83466 REFERENCES IN FILE CAPLUS (1967 TO DATE)

Finding RN's for Polymers



Registry Search Fields

Search Field	Field Code	Example
CAS Registry Number	**/RN (or none)**	**S 29035-74-3**
Component Registry Number	**/CRN**	**S 110-63-4/CRN**
Chemical Name	**/CN**	**S POLYSTYRENE/CN**
Molecular Formula	**/MF**	**S "(C8H8)X"/MF**
Number of Components	**/NC**	**S L1 AND 2/NC**
Polymer Class Term	**/PCT**	**S POLYSTYRENE/PCT**

Finding Polymers by Name

```
=> E VINYL CHLORIDE POLYMER/CN
E1    1      VINYL CHLORIDE OCTAMER/CN
E2    1      VINYL CHLORIDE PENTAMER/CN
E3    1 --> VINYL CHLORIDE POLYMER/CN
E4    1      VINYL CHLORIDE RADICAL CATION/CN
E5    1      VINYL CHLORIDE RESIN/CN
E6    1      VINYL CHLORIDE RUBBER/CN
E7    1      VINYL CHLORIDE SYNTHETIC RUBBER/CN
E8    1      VINYL CHLORIDE TETRAMER/CN
E9    1      VINYL CHLORIDE TRIMER/CN
O O O

=> S E3
L1             1 "VINYL CHLORIDE POLYMER"/CN
```

Finding Polymers by Name

```
=> D

L1    ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2002 ACS
RN    9002-86-2  REGISTRY
CN    Ethene, chloro-, homopolymer (9CI)
(CA INDEX NAME)
OTHER NAMES:
CN    1000Z
CN    101EP
CN    1032X
O O O
CN    Amerace A 30
CN    Vinyl chloride polymer
O O O
```

Finding Polymers by CRN

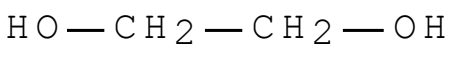
- **Step 1** Find the RN for each monomer.
- **Step 2** Search RN in the Component Registry Number (/CRN) field.
- **Step 3** Combine using AND operator.
- **Step 4** Limit by Number of Components (/NC) field.

Finding Polymers by CRN

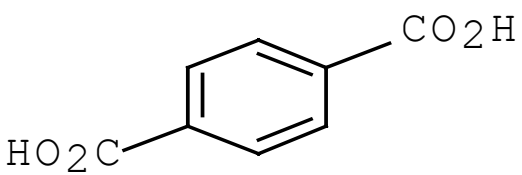
```
=> FIL REG

=> S 1,4-BENZENEDICARBOXYLIC ACID/CN
L1             1 1,4-BENZENEDICARBOXYLIC ACID/CN

=> D
L1   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2002 ACS
RN   100-21-0  REGISTRY
CN   1,4-Benzenedicarboxylic acid (9CI)    (CA INDEX NAME)
O O O

=> S 1,2-ETHANEDIOL/CN
L2             1 1,2-ETHANEDIOL/CN

=> D L2
L2   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2002 ACS
RN   107-21-1  REGISTRY
CN   1,2-Ethanediol (9CI)    (CA INDEX NAME)
O O O
```

Finding Polymers by CRN

```
=> S L3 AND 2/NC
        2620877 2/NC
L4              5 L3 AND 2/NC

=> D SCAN
L4  5 ANSWERS   REGISTRY  COPYRIGHT 2002 ACS
IN  1,4-Benzenedicarboxylic acid, polymer with 1,2-ethanediol(9CI)
MF  (C8 H6 O4 . C2 H6 O2)x
CI  PMS, COM

    CM   1
```



```
    CM   2
```



```
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):END
```

Finding Polymers by PCT

Polymer class terms (PCT's) describe broad classes of polymers. The current REGISTRY PCT's are:

AMINO RESIN
CHLOROPOLYMER
DOUBLE STRAND
EPOXY RESIN
FLUOROPOLYMER
MANUAL COMPONENT
MANUAL REGISTRATION
OTHER
PHENOLIC RESIN
POLYACETYLENE
POLYACRYLIC
POLYAMIC ACID
POLYAMIDE
POLYAMINE
POLYANHYDRIDE
POLYAZOMETHINE
POLYBENZIMIDAZOLE
POLYBENZOXAZOLE
POLYCARBODIIMIDE
POLYCARBONATE
POLYCYANURATE
POLYESTER
POLYHYDRAZIDE
POLYIMIDE
POLYIONENE
POLYISOCYANURATE
POLYKETONE
POLYNUCLEOTIDE
POLYOLEFIN
POLYOTHER
POLYPHENYL
POLYPHOSPHAZENE
POLYQUINOXALINE
POLYSTYRENE
POLYSULFIDE
POLYSULFONAMIDE
POLYSULFONE
POLYTHIOESTER
POLYTHIOETHER
POLYUREA
POLYURETHANE
POLYVINYL

Finding Polymers by PCT

```
=> FIL REG

=> S FLUOROPOLYMER/PCT
L1          8566 FLUOROPOLYMER/PCT

=> FIL HCAPLUS

=> S L1
L2         61224 L1
```

Polymer Terms in HCAplus

```
=> E FLUOROPOLYMERS/CT
E#    FREQUENCY     AT      TERM
--    ---------     --      ----
E1            0      1      FLUOROPOLYMER-URETHANE/CT
E2            0      3      FLUOROPOLYMER-URETHANE FIBERS/CT
E3        42833    245 --> FLUOROPOLYMERS/CT
E4            0      5      FLUOROPOLYMERS (L)  O O O

=> E E3+NT1/CT
E1        42833    -->  Fluoropolymers/CT
                        NOTE Polymers having a C-F bond in the
                             repeating portion of
                             the chain are indexed here.
E2            0      NT1  Chlorotrifluoroethylene-ethylene
                             copolymer/CT
E3            0      NT1  Chlorotrifluoroethylene-vinylidene
                             fluoride copolymer/CT
E4            0      NT1  Ethylene-tetrafluoroethylene copolymer/CT
E5         1746    **NT1  Fluoro rubber/CT
O O O
```

Polymer Terms in HCAplus

```
=> S E3+ALL
L3          206035 FLUOROPOLYMERS+ALL/CT   (245 TERMS)

=> S L2 OR L3
L4          208494 L2 OR L3

=> S L4(L)ANTIFRICTION COATING#
L5              83 L4(L)ANTIFRICTION COATING#
```

Polymer Terms in HCAplus

```
=> D HIT

L5   ANSWER 1 OF 83  CAPLUS  COPYRIGHT 2002 ACS
IT   Fluoro rubber
     RL: PRP (Properties); TEM (Technical or engineered material
      use); USES
     (Uses)
        (chlorotrifluoroethylene-vinylidene fluoride, SKF 32;
        antifriction  coatings  from fluoro rubber vulcanized
        under laser radiation)
IT   9010-75-7 , Chlorotrifluoroethylene-vinylidene fluoride
     copolymer
     RL: PRP (Properties); TEM (Technical or engineered material
use); USES
     (Uses)
        (rubber; antifriction  coatings  from fluoro
        rubber vulcanized under laser radiation)
```

Finding Polymer Properties

```
=> E MECHANICAL PROPERTIES+NT1/CT
E1          6833    -->  Mechanical properties/CT
E2             1      NT1  Active crystal length/CT
E3             1      NT1  Active slip volume/CT
E4           410      NT1  Anelasticity/CT
E5          1069      NT1  Brittleness/CT
E6            90      NT1  Bulk modulus/CT
E7            39      NT1  Cleavage/CT
E8          2980    **NT1  Compressibility/CT
O O O
E15        14585    **NT1  Elasticity/CT
E16         1013    **NT1  Electromechanical effect/CT
E17          649      NT1  Flexibility/CT
O O O
E37         4468    **NT1  Toughness/CT
*********  END***
```

Finding Polymer Properties

```
=> INDEX PLASDATA
INDEX 'ASMDATA, PDLCOM, PLASPEC' ENTERED
3 FILES IN THE FILE LIST IN STNINDEX

=> S NOVADOWL
0 FILES HAVE ONE OR MORE ANSWERS,3 FILES SEARCHED IN STNINDEX
L1    QUE NOVADOWL

=> FIL REG

=> S L1
L2             1 NOVADOWL

=> D
L2    ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2002 ACS
RN    26062-94-2  REGISTRY
CN    1,4-Benzenedicarboxylic acid, polymer with
      1,4-butanediol (9CI)  (CA INDEX NAME)
```

Finding Polymer Properties

```
=> SEL CHEM
E1 THROUGH E25 ASSIGNED

=> DIS SEL
E1              1      BUTANEDIOL-TEREPHTHALIC ACID COPOLYMER/BI
E2              1      BUTYLENE GLYCOL-TEREPHTHALIC ACID
                        COPOLYMER/BI
E3              1      BUTYLENE GLYCOL-TEREPHTHALIC ACID
                        POLYMER/BI
E4              1      NOVADOWL/BI
O O O
E25             1      26062-94-2/BI

=> FIL PLASPEC

=> S E1-E25
```

Finding Polymer Properties

```
=> D ALL

L8   ANSWER 1 OF 330  PLASPEC  COPYRIGHT 2002 BCI
Database: PLASPEC/Manufacturer's Data   AN: 400-21735
Material Class:         Thermoplastic
Family Name:            Polybutylene terephthalate
Trade Name and Grade:   Crastin S660FR
CAS Registry Number:    24968-12-5 (Polybutylene terephthalate)
                        26062-94-2 (Polybutylene terephthalate)
Resin Form:             pellets
Supplier:               DuPont Engineering Polymers
Application:            Electrical
Features:               Flame retardant
```

Finding Polymer Properties

Processing/Physical Characteristics

Process Type:	Injection molding
Recommended Melt Temperature:	464 - 500 deg F
Density:	1.45 g/cm**3 at ambient temperature
Shrinkage, Mold:	1.8 in/in in machine direction
	2.2 in/in in transverse direction
Water Absorption, 24 Hour:	0.06%

Mechanical Properties

Elongation at Break:	10%
Flexural Yield Strength:	1.17E+04 psi
Compressive Ultimate Strength:	1.06E+04 psi
Modulus of Elasticity	
Tensile:	4.3E+05 psi
Flexural:	3.9E+05 psi

Finding Polymer Properties

Hardness	
Rockwell:	**R116**
Izod Impact Energy, Normalized:	**0.8 ft*lbf/in for 0.125 in wide specimen**
Thermal Properties	
Melting Point:	**437 deg F**
Linear Expansion Coefficient:	**7E-05 in/in*deg F**
Electrical Properties	
Dielectric Strength	
Short Time:	**400 V/mil**
Dielectric Constant:	**3 at 60 Hz**
Volume Resistivity:	**1E+16 ohm*cm**
Surface Resistivity:	**5E+14 ohm**